This week in techniques

Approach	Summary	Licensing status	Publication and contact information
Computational models			
Computational algorithm for designing G protein-coupled receptor (GPCR) ligands against a predefined set of targets	<p>A computational algorithm could be used to design GPCR ligands that modulate a predefined set of targets. Starting from Aricept donepezil, which has moderate dopamine D4 receptor activity and low dopamine D2 receptor activity, an automated algorithm predicted compounds that would have increased D2 receptor activity and blood brain barrier (BBB) permeability. The eight highest-ranked molecules all retained D4 receptor activity and had greater D2 receptor affinity than Aricept, and one compound tested in mice also penetrated the BBB. Next steps include determining whether the method can be used for lead optimization and applied to other target families.</p> <p>Pfizer Inc. and Eisai Co. Ltd. market the acetylcholinesterase (AChE) inhibitor Aricept for Alzheimer's disease (AD).</p> <p>SciBX 6(2); doi:10.1038/scibx.2013.43 Published online Jan. 17, 2013</p>	Patented; licensed to Ex Scientia Ltd.	<p>Besnard, J. <i>et al. Nature</i>; published online Dec. 12, 2012; doi:10.1038/nature11691</p> <p>Contact: Andrew L. Hopkins, University of Dundee, Dundee, U.K. e-mail: a.hopkins@dundee.ac.uk</p>